IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

Applicant:	Harold E. Helson	Confirmation No.:	4787
Application No.:	09/502,133	Art Unit:	2128
Filed:	February 11, 2000	Examiner:	H. M. Jones
Title:	ENHANCING STRUCTURE DIAGRAM GENERATION		

Commissioner for Patents
P.O. Box 1450
Alexandria, VA 22313-1450

DECLARATION UNDER 37 C.F.R. § 1.132

Dear Sir:

I, Dr. Christoph Steinbeck, declare as follows.

1. I have studied and worked in the areas of general and computational chemistry since 1993. I have contributed to the field of SDG. I have studied chemistry and received a phd in chemistry in 1995 from the University of Bonn, Germany. After a postdoctorate at Tufts University in Boston, MA, USA and group leaderships in Jena and Cologne (both in Germany) I am now head of cheminformatics and metabolism at the European Bioinformatics Institute in Hinxton, Cambridge, Uk, and currently editor-in-chief of the Journal of Cheminformatics.

2. I have reviewed the above-identified application (the '133 Application herein) and the Office Action issued by the Examiner dated May 25, 2010, for the '133 Application.

3. I have been informed that pending claims 1, 9, and 13-35 have been rejected in the latest Office Action under 35 U.S.C. § 103(a) as purportedly being unpatentable over Helson, "Simulation of Carbene Chemistry and Other Problems in Computer-Assisted Organic Synthesis", Purdue

University 1993 (herein Helson) in view of Benecke, C., *et al.*, "MOLGEN+, a generator of connectivity isomers and stereoisomers for molecular structure elucidation", *Anal. Chim. Acta*, Vol. 314, pp. 141-147, 1995 (herein Benecke) and the taking of official notice. Specifically, I have been informed that Benecke has been alleged to disclose the laying out of atoms and/or bonds to express symmetry. In addition, I have been informed that the latest Office Action states that, "*Laying out the symmetrically equivalent atoms and bonds* by itself means that the symmetries are expressed." (Emphasis in the original.)

4. I have read and understood Benecke.

5. Benecke describes a structure generator software application, MOLGEN+, which produces all of the molecular graphs that correspond to a given chemical formula. As disclosed in Benecke, MOLGEN+ takes as its input a chemical formula, (optionally) prescribed and forbidden substructures, an interval for allowed ring sizes, and maximal bond multiplicities. From this input, MOLGEN+ generates a complete list of all mathematically possible molecular graphs that are compatible with the chemical formula. After generation of the constitutional isomers, MOLGEN+ produces a sketch of the molecules in the form of a tapestry of several molecules shown together or as a single molecule.

6. In my opinion, one having ordinary skill in the art of computer-based chemical structure diagram generation would not understand Benecke as disclosing or suggesting "determining an arrangement of chemically symmetrically equivalent atoms and bonds to provide a visually symmetric expression of an identified chemical structural symmetry" or "laying out the chemically symmetrically equivalent atoms and bonds in a two-dimensional pictorial representation of the chemical structure in accordance with the determined arrangement."

7. Benecke states, "MOLGEN+ is capable of generating all possible configurational isomers, again redundancy free (which also implies the consideration of symmetries)." In my opinion, one having skill in the art of computer-based chemical structure diagram generation would understand

this statement to mean that symmetries were considered only to avoid duplications and missing objects when generating all permutations of a list of elements.

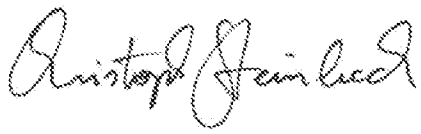
8. The invention being claimed in the '133 Application requires identifying an instance of chemical structural symmetry in a chemical structure, determining an arrangement of chemically symmetrically equivalent atoms and bonds to provide a visually symmetric expression of an identified chemical structural symmetry, and laying out the chemically symmetrically equivalent atoms and bonds in a two-dimensional pictorial representation of the chemical structure in accordance with the determined arrangement. Thus, it is a method that requires certain steps to be completed. In particular, the claimed method requires intentional contemplation of chemical structural symmetry in the determination of how a chemical structure is to be visually expressed.

9. In my opinion, the claimed invention would not be obvious in light of Helson and Benecke because the combined references do not teach or suggest determining an arrangement of chemically symmetrically equivalent atoms and bonds to provide a visually symmetric expression of an identified chemical structural symmetry and laying out the chemically symmetrically equivalent atoms and bonds in a two-dimensional pictorial representation of the chemical structure in accordance with the determined arrangement.

10. In my opinion, one having ordinary skill in the art of computer-based chemical structure diagram generation and reading the specification of the '133 Application would understand the specific technique for adding symmetry as a parameter in dynamic ring layout described on page 10, line 12 through page 13, line 6 as a non-limiting illustrative example of determining an arrangement of chemically symmetrically equivalent atoms and bonds to provide a visually symmetric expression of an identified chemical structural symmetry.

11. I am familiar with structure drawing software at and after the date of filing of this patent (2000). To the best of my knowledge, no product at that time intentionally expressed chemical structural symmetry in a visually symmetric manner. In my opinion, this feature was an advance over the state of the art of structure diagram generation at that time.

12. I hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements are made with the knowledge that willful false statements so made are punishable by fine or imprisonment or both under § 1001 of Title 18 of the United States Code and that such willful statements may jeopardize the validity or enforceability of the present application or any patent issued thereon.



21 November 2010

Dr. Christoph Steinbeck Date